

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom

10/644,076

=> d his

(FILE 'HOME' ENTERED AT 10:17:48 ON 10 FEB 2006)

FILE 'REGISTRY' ENTERED AT 10:17:53 ON 10 FEB 2006

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 118 S L1 SSS FUL

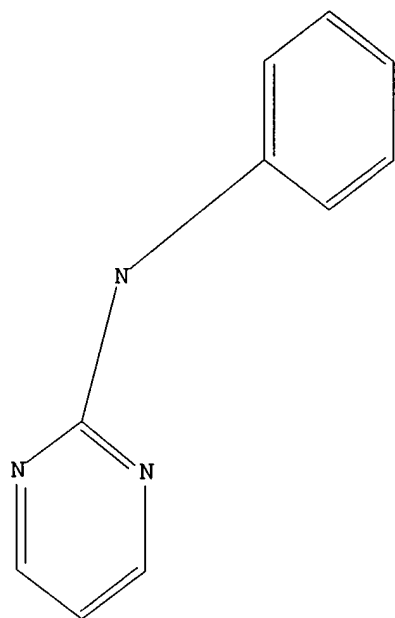
FILE 'CAPLUS' ENTERED AT 10:18:23 ON 10 FEB 2006

L4 15 S L3

=> d l1

L1 HAS NO ANSWERS

L1 STR

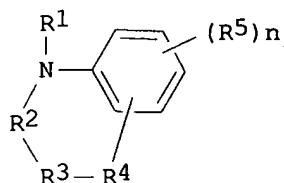


Structure attributes must be viewed using STN Express query preparation.

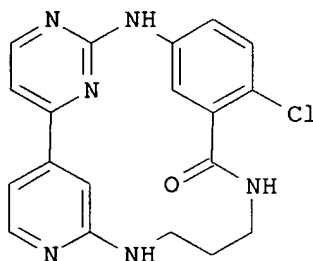
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ANSWER 1 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2004:756664 CAPLUS
 DOCUMENT NUMBER: 141:243576
 TITLE: Preparation of macrocycle amino compounds and compositions as cyclin-dependent protein kinase inhibitors
 INVENTOR(S): Ren, Pingda; Adrian, Francisco; Gray, Nathanael S.; Wang, Xia
 PATENT ASSIGNEE(S): IRM LLC, Bermuda
 SOURCE: PCT Int. Appl., 40 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078682	A2	20040916	WO 2004-US6947	20040305
WO 2004078682	A3	20051208		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2004235841	A1	20041125	US 2004-794454	20040305
PRIORITY APPLN. INFO.:			US 2003-452633P	P 20030305
OTHER SOURCE(S):			MARPAT 141:243576	
GI				



I



II

AB The invention provides a novel class of cyclic compds. I, wherein n is 0-3; R¹ hydrogen and alkyl; R²-R³ are independently substituted arylene and hetero-arylene; R⁴ is -XIR⁶(CH₂)_mNR⁷C(O)-, -XNR⁶(CH₂)_mNR⁷C(O)CH₂-, -XR⁶(CH₂)_mNR⁷(CH₂)_mNR⁷C(O)-, -O(CH₂)_mNR⁷C(O)-, -NR⁶(CH₂)_mO- and -XNR⁶(CH₂)_mNR⁷CH₂-; wherein X is a bond or C-alkylene; m is 1-6; R⁶ and R⁷ independently are hydrogen and alkyl; and R⁵ is halo, alkyl, halo-substituted alkyl, alkoxy and halo-substituted alkoxy and

heterocycloalkyl; wherein any heterocycloalkyl of R5 is substituted with a group halo, alkyl, halo-substituted alkyl, alkoxy, halo-substituted alkoxy, heterocycloalkyl-alkyl and -XNR8R9, wherein X is a bond or alkylene; R8 and R9 are independently hydrogen and alkyl; or a salt thereof pharmaceutical compns. comprising such cyclic compds. and methods of using such compds. to treat or prevent diseases and disorders associated with cyclin-dependent kinases (CDKs) activity, particularly diseases associated with the activity of CDK2 and CDK5. Thus, macrocycle II was prepared and tested as CDK2 and CDK5 inhibitors.

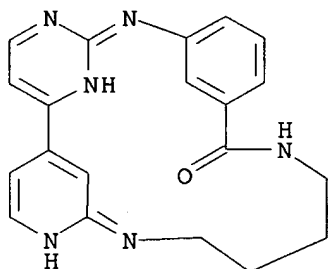
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 752245-26-4P 752245-27-5P 752245-28-6P
 752245-29-7P 752245-30-0P 752245-31-1P
 752245-32-2P 752245-36-6P 752245-37-7P
 752245-38-8P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of macrocycle amino compds. and compns. as cyclin-dependent protein kinase inhibitors)

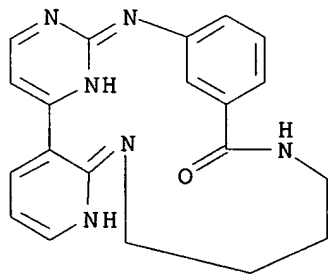
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RN 752245-05-9 CAPLUS

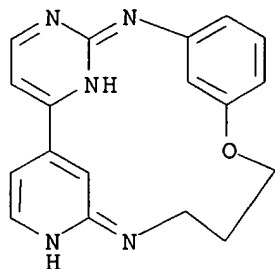
CN 7H,13H-8,12-Metheno-14,18-nitrilopyrido[3,2-g][1,3,9,14]tetraazacycloeicosin-7-one, 1,2,3,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



10/644,076

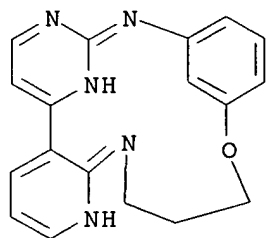
RN 752245-06-0 CAPLUS

CN 13-Oxa-5,7,17,19,24-pentaazatetracyclo[16.3.1.12,6.18,12]tetracos-
1(22),2,4,6(24),8,10,12(23),18,20-nonaene (9CI) (CA INDEX NAME)



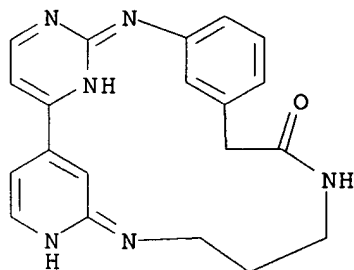
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CN 11H-6,10-Metheno-12,16-nitrilo-10H-pyrido[2,3-
f][1,5,11,13]oxatriazacyclooctadecine, 1,2,3,4-tetrahydro- (9CI) (CA
INDEX NAME)



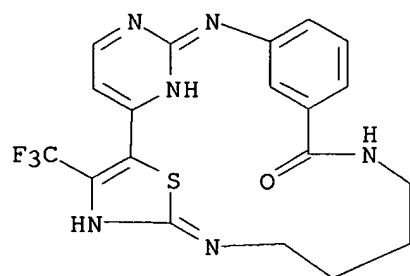
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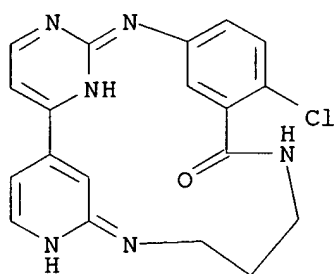


RN 752245-09-3 CAPLUS

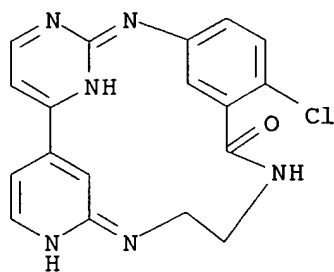
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(CA INDEX NAME)



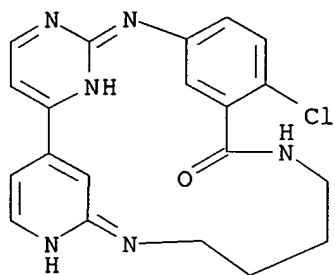
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 INDEX NAME)



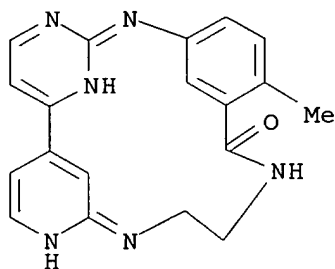
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 INDEX NAME)



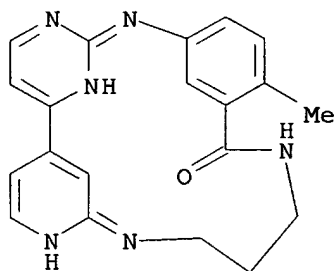
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 INDEX NAME)



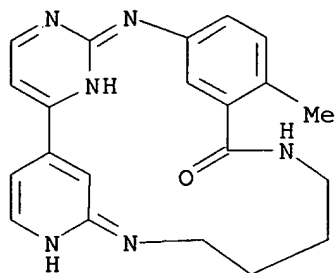
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 INDEX NAME)



RN 752245-14-0 CAPLUS
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 INDEX NAME)

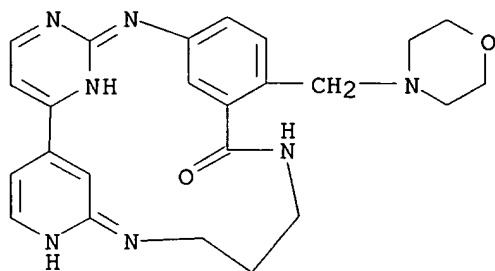


RN 752245-15-1 CAPLUS
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 INDEX NAME)



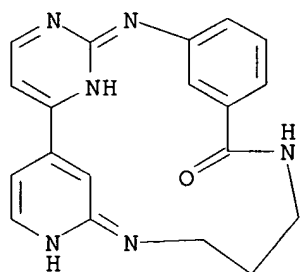
RN 752245-16-2 CAPLUS

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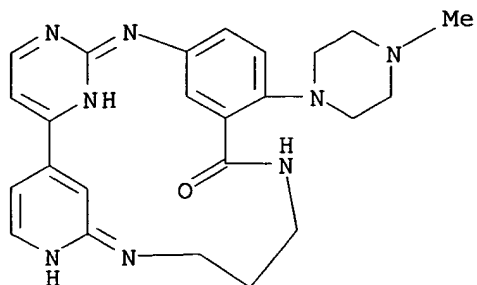
RN 752245-17-3 CAPLUS

CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosane-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one (9CI) (CA INDEX NAME)



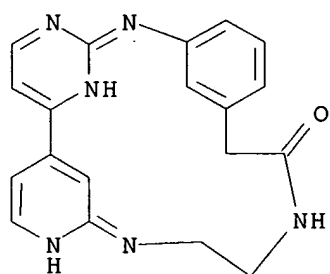
RN 752245-18-4 CAPLUS

CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosane-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one, 11-(4-methyl-1-piperazinyl)-(9CI) (CA INDEX NAME)



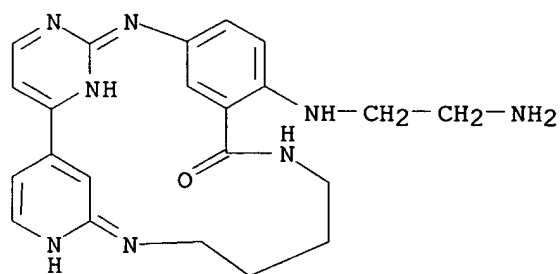
RN 752245-19-5 CAPLUS

CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-
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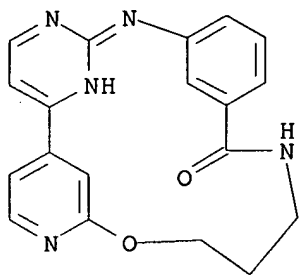
RN 752245-20-8 CAPLUS

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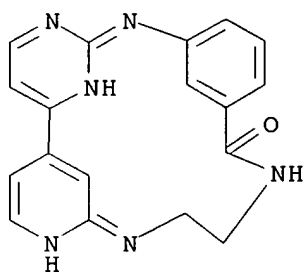


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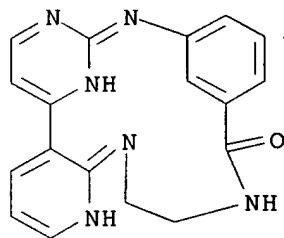
CN 18-Oxa-5,7,14,20,25-pentaazatetracyclo[17.3.1.12,6.18,12]pentacosa-
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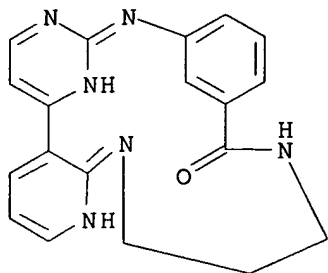
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RN 752245-24-2 CAPLUS
 CN 5H,11H-6,10-Metheno-12,16-nitrilopyrido[3,2-g][1,3,9,12]tetraazacyclooctadec-5-one, 1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

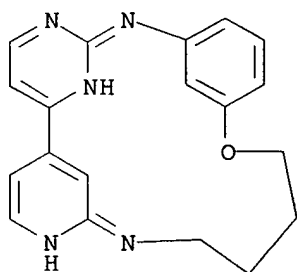


RN 752245-25-3 CAPLUS
 CN 7,11-Metheno-13,17-nitrilo-12H-pyrido[3,2-g][1,3,9,13]tetraazacyclononadec-6(1H)-one, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



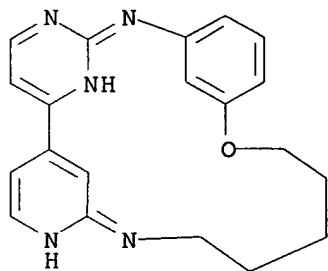
RN 752245-26-4 CAPLUS

CN 13-Oxa-5,7,18,20,25-pentaazatetracyclo[17.3.1.12,6.18,12]pentacosal-1(23),2,4,6(25),8,10,12(24),19,21-nonaene (9CI) (CA INDEX NAME)



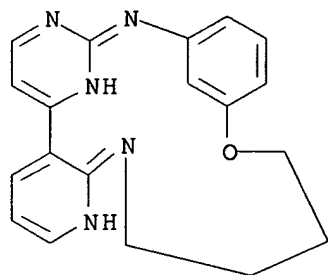
RN 752245-27-5 CAPLUS

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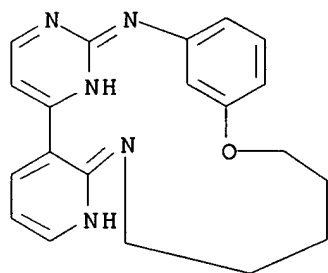


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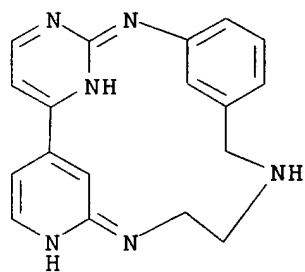
CN 1H,12H-7,11-Metheno-13,17-nitrilopyrido[2,3-g][1,6,12,14]oxatriazacyclononadecine, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



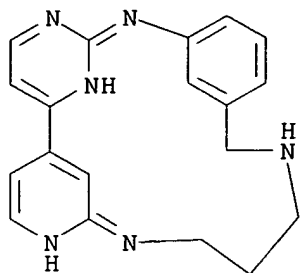
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 INDEX NAME)



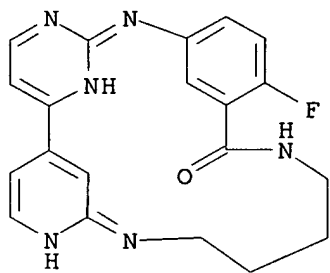
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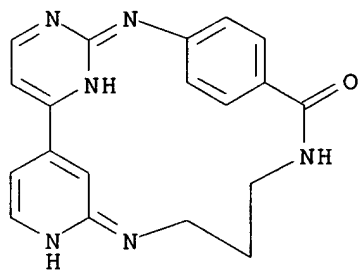
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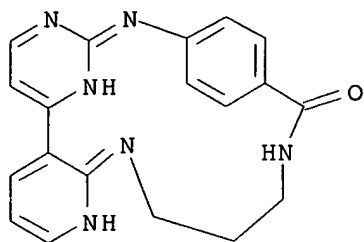
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 INDEX NAME)



RN 752245-36-6 CAPLUS
 CN 2,4,11,13,17,25-Hexaazatetracyclo[17.2.2.13,7.18,12]pentacosa-
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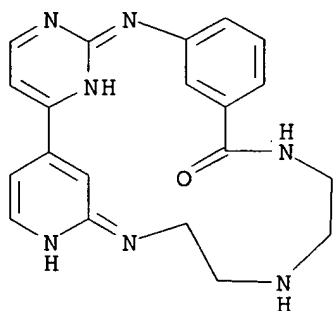


RN 752245-37-7 CAPLUS
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 6(11H)-one, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



RN 752245-38-8 CAPLUS

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1(25),2,4,6(27),8,10,12(26),21,23-nonaen-13-one (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:177944 CAPLUS

DOCUMENT NUMBER: 140:235737

TITLE: Production of macrocyclic pyrimidine derivatives and their use as drugs

INVENTOR(S): Luecking, Ulrich; Siemeister, Gerhard; Schaefer, Martina; Briem, Hans

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 42 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10239042	A1	20040304	DE 2002-10239042	20020821
CA 2492319	AA	20040401	CA 2003-2492319	20030805
WO 2004026881	A1	20040401	WO 2003-EP8664	20030805
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1530574	A1	20050518	EP 2003-797225	20030805
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012874	A	20050628	BR 2003-12874	20030805
JP 2006501271	T2	20060112	JP 2004-536924	20030805
US 2004209895	A1	20041021	US 2003-644076	20030820
NO 2005001448	A	20050318	NO 2005-1448	20050318
PRIORITY APPLN. INFO.:			DE 2002-10239042	A 20020821
			US 2002-413444P	P 20020926
			WO 2003-EP8664	W 20030805
OTHER SOURCE(S):		CASREACT 140:235737; MARPAT 140:235737		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Macrocyclic pyrimidine derivs., e.g., I [R1, R5 = H, OH, halogen, NO2, CN, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R2 = H, C1-10-alkyl; R3 = H, halogen, NO2, CN, C1-10-alkyl, C1-10-haloalkyl, C2-10-alkenyl, C2-10-alkynyl, C2-10-cycloalkyl, OH, C1-6-alkoxy, C1-6-alkylthio, NH2, NH(CH2)p-C3-10-cycloalkyl, C1-6-hydroxyalkyl, (C1-6-alkoxy)-(C1-6-alkyl), NH(C1-6-alkyl), N(C1-6-alkyl)2, SO(C1-6-alkyl), SO2(C1-6-alkyl), (C1-6-alkanoyl), CONR8R9, COR10, (C1-6-alkyl)-OAc, CO2H, aryl, heteroaryl, etc.; R4 = H, halogen, C1-4-alkyl; R6, R7, R8, R9, R10, R11 = H, OH, halogen, C1-12-alkoxy, C1-6-alkylthio, NH2, CN, C1-6-alkyl, NH(CH2)p-C3-10-cycloalkyl,

C3-10-cycloalkyl, C1-6-hydroxyalkyl, C2-6-alkenyl, C2-6-alkynyl, NH-(C1-6-alkyl), N(C1-6-alkyl)₂, SO(C1-6-alkyl), SO₂(C1-6-alkyl), C1-6-alkanoyl, CONR₈R₉, etc.; X, Y = O, S, NR₁₁, NR₁₁O, ONR₁₁, CR₆R₇, C:O, C:S, SO, SO₂, C(:O)O, OC(:O), S(:O)O, OS(:O), SO₂-O, O-SO₂, CONR₈, NR₈CO, OC(:O)NR₈, NR₈C(:O)O, CSNR₈, NR₈CS, OC(:S)NR₈, SONR₈, NR₈SO, SO₂NR₈, NR₈SO₂, NR₈COR₉, NR₈CSNR₉, NR₈SONR₉, NR₈SO₂NR₉, NR₈CONR₉, NR₈CSNR₉; A = aryl, heteroaryl; B = bond; m = 0 - 8; n, p = 0 - 6], II (D = NH₂, NO₂) and III (U = OH), their isomers, stereoisomers, enantiomers and their salts, which are inhibitors of the cyclin-dependent kinases, procedures for their production as well as their use as medicine for the treatment of different illnesses is described. Preparation of I is characterized by macrocyclization of pyrimidine IV (L = leaving group) in the presence of an acid and is itself prepared via reduction of nitro compound V (L = leaving group). Thus, I [R₁ = R₂ = R₄ = R₅ = H, R₃ = Br, A = 1,3-phenylene, (Y)_nB(X)_n = NH(CH₂)₅NHSO₂, m = n = 1] was prepared via macrocyclization of IV [L = Cl, R₁ = R₂ = R₄ = R₅ = H, R₃ = Br, A = 1,3-phenylene, (Y)_nB(X)_n = NH(CH₂)₅NHSO₂, m = n = 1]. The inhibitory activity of I [R₁ = R₂ = R₄ = R₅ = H, R₃ = Br, A = 1,3-phenylene, (Y)_nB(X)_n = NH(CH₂)₅NHSO₂, m = n = 1] towards cyclin-dependent kinases was determined [IC₅₀ = 420 nM vs. CDK1/CycB, IC₅₀ = 200 nM vs. CDK2/CycE, IC₅₀ = 1.1 nM vs. MCF7].

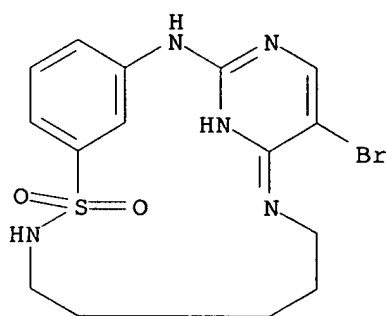
IT 666719-26-2P 666719-27-3P 666719-28-4P
666719-29-5P 666719-30-8P 666719-32-0P
666719-34-2P 666719-35-3P 666719-36-4P
666719-37-5P 666719-38-6P 666719-39-7P
666719-40-0P 666719-41-1P 666719-42-2P
666719-43-3P 666719-44-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of macrocyclic pyrimidine derivs. which are inhibitors of the cyclin-dependent kinases)

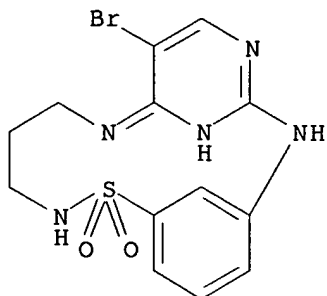
RN 666719-26-2 CAPLUS

CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene, 6-bromo-, 15,15-dioxide (9CI) (CA INDEX NAME)

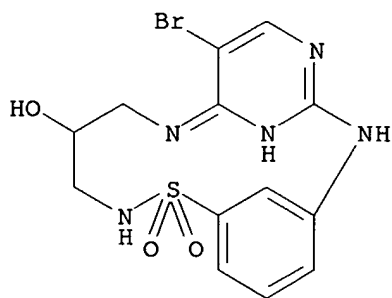


RN 666719-27-3 CAPLUS

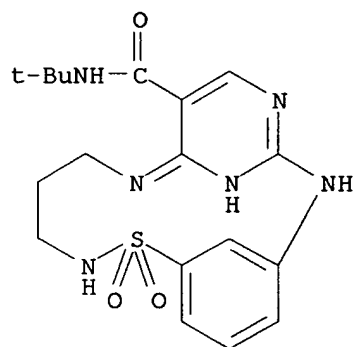
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo-, 13,13-dioxide (9CI) (CA INDEX NAME)



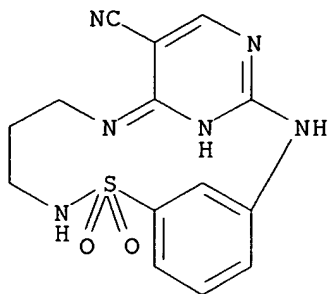
RN 666719-28-4 CAPLUS
 CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-
 1(18),2,4,6,14,16-hexaen-10-ol, 6-bromo-, 13,13-dioxide (9CI) (CA INDEX
 NAME)



RN 666719-29-5 CAPLUS
 CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-
 1(18),2,4,6,14,16-hexaene-6-carboxamide, N-(1,1-dimethylethyl)-,
 13,13-dioxide (9CI) (CA INDEX NAME)

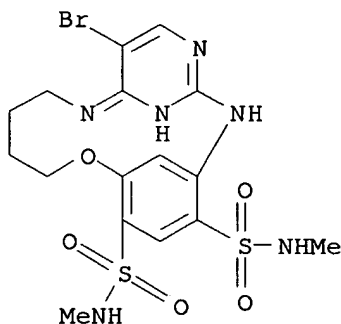


RN 666719-30-8 CAPLUS
 CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-
 1(18),2,4,6,14,16-hexaene-6-carbonitrile, 13,13-dioxide (9CI) (CA INDEX
 NAME)



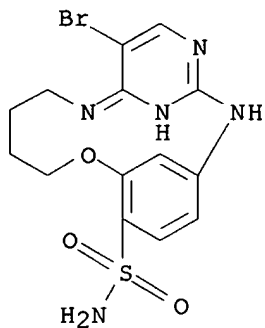
RN 666719-32-0 CAPLUS

CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),3,5,7(19),14,16-hexadecaene-15,17-disulfonamide, 6-bromo-N,N'-dimethyl- (9CI) (CA INDEX NAME)



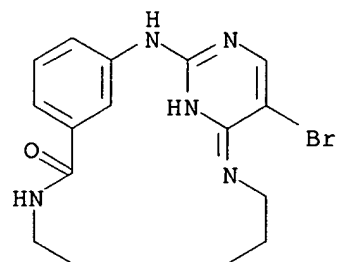
RN 666719-34-2 CAPLUS

CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene-15-sulfonamide, 6-bromo- (9CI) (CA INDEX NAME)

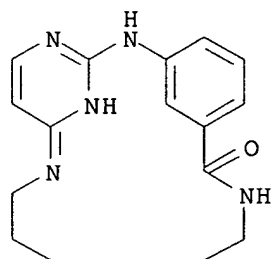


RN 666719-35-3 CAPLUS

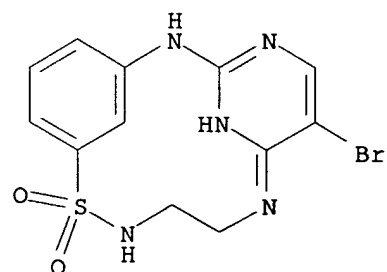
CN 2,4,8,14,21-Pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaen-15-one, 6-bromo- (9CI) (CA INDEX NAME)



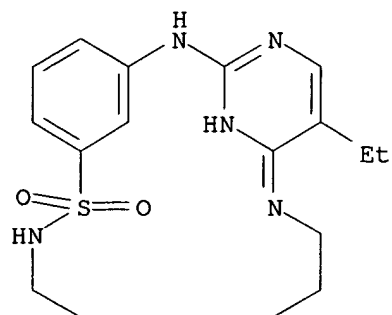
RN 666719-36-4 CAPLUS
 CN 2,4,8,14,21-Pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaen-15-one (9CI) (CA INDEX NAME)



RN 666719-37-5 CAPLUS
 CN 12-Thia-2,4,8,11,18-pentaazatricyclo[11.3.1.13,7]octadeca-1(17),2,4,6,13,15-hexaene, 6-bromo-, 12,12-dioxide (9CI) (CA INDEX NAME)

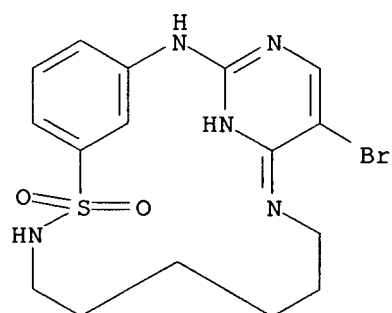


RN 666719-38-6 CAPLUS
 CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene, 6-ethyl-, 15,15-dioxide (9CI) (CA INDEX NAME)



RN 666719-39-7 CAPLUS

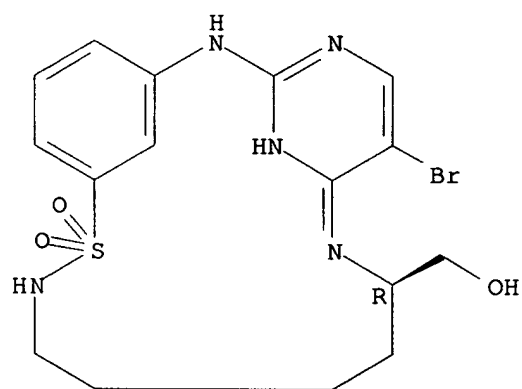
CN 16-Thia-2,4,8,15,22-pentaazatricyclo[15.3.1.13,7]docosa-1(21),2,4,6,17,19-hexaene, 6-bromo-, 16,16-dioxide (9CI) (CA INDEX NAME)



RN 666719-40-0 CAPLUS

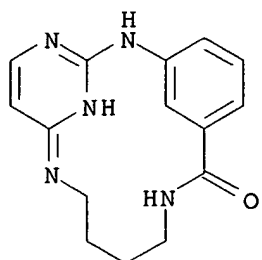
CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene-9-methanol, 6-bromo-, 15,15-dioxide, (9R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



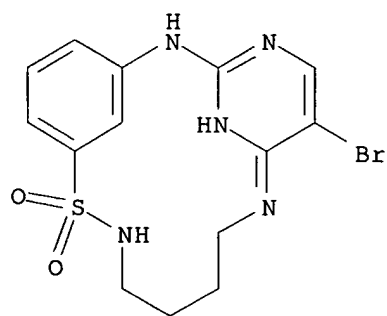
RN 666719-41-1 CAPLUS

CN 2,4,8,13,20-Pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaen-14-one (9CI) (CA INDEX NAME)



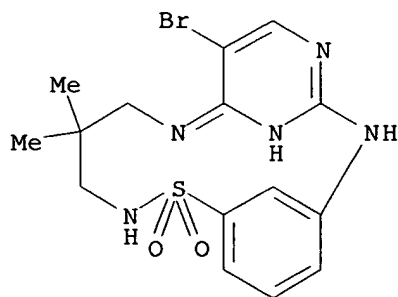
RN 666719-42-2 CAPLUS

CN 14-Thia-2,4,8,13,20-pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaene, 6-bromo-, 14,14-dioxide (9CI) (CA INDEX NAME)



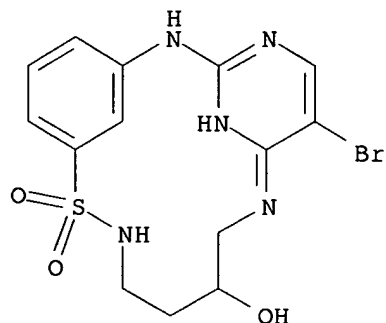
RN 666719-43-3 CAPLUS

CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo-10,10-dimethyl-, 13,13-dioxide (9CI) (CA INDEX NAME)



RN 666719-44-4 CAPLUS

CN 14-Thia-2,4,8,13,20-pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaen-10-ol, 6-bromo-, 14,14-dioxide (9CI) (CA INDEX NAME)

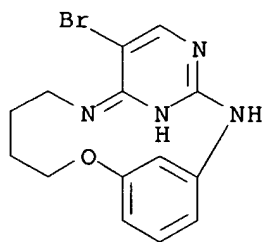


IT **666719-33-1P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, aminosulfonylation and inhibition by, of cyclin-dependent kinases; preparation of macrocyclic pyrimidine derivs. which are inhibitors of the cyclin-dependent kinases)

RN 666719-33-1 CAPLUS

CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:737797 CAPLUS

DOCUMENT NUMBER: 132:85803

TITLE: Light-sensitive methacrylic acid based copolymers containing the 2-(2-chloroanilino)-4,6-dimethylpyrimidine chromophore in the side chain

AUTHOR(S): Lebedeva, G. K.; Ivanova, V. N.; Denisov, V. M.; Kudryavtsev, V. V.; Frolov, A. N.

CORPORATE SOURCE: Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg, Russia

SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (1999), 69(6), 981-985
CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

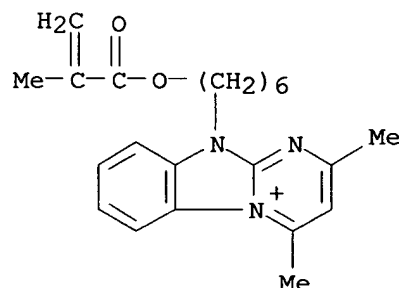
AB New light-sensitive copolymers containing the o-chlorophenylpyrimidine chromophore in the side chain were prepared and studied. The ¹H NMR and electronic spectra, interpreted using model compds., showed that the main photochem. reaction of the copolymers is cyclization at the heterocyclic nitrogen atom of the o-chloropyrimidinium chromophore to give N-substituted pyrimido[1,2-a]benzimidazolium chromophore.

IT 253662-25-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (photoproduct; photolysis of (dimethylpyrimidyl)(chlorophenyl)aminohexyl methacrylate in relation to photolysis of methacrylate copolymers containing chlorophenylpyrimidine chromophore in side chain)

RN 253662-25-8 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-dimethyl-10-[6-[(2-methyl-1-oxo-2-propenyl)oxy]hexyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L4~~ ANSWER 4 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:570215 CAPLUS

DOCUMENT NUMBER: 131:322704

TITLE: Direct cycloauration of 1-(2-pyridylamino and 2-pyrimidinylamino)naphthalene and 2-(p-toluidino)quinoline with sodium tetrachloroaurate(III)

AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Nagoya, 464-8602, Japan

SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands) (1999), 24(4), 449-453

CODEN: TMCHDN; ISSN: 0340-4285

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

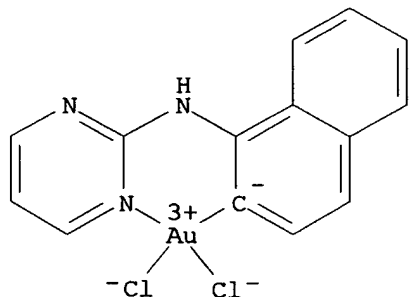
AB 1-(2-Pyridylamino and 2-pyrimidinylamino)naphthalene (abbreviated as Hpyn and Hpnm, resp.) and 2-(p-toluidino)quinoline (Htlq) were directly cycloaurated with Na[AuCl₄] to give [AuCl₂L] (L = pyn, pmn, or tlq). These complexes were characterized spectroscopically and the square planar structure of [AuCl₂(pmn)] was determined by x-ray anal. The naphthalene ring was aurated at position 2, forming a six-membered auraheterocycle with concomitant coordination of the pyrimidine-N atom. The trans influence of the C donor was clearly reflected in the AuCl bond lengths; 2.372(2) trans to C and 2.275 Å trans to N. Similar square planar structures were suggested for the other two complexes.

IT 248937-34-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure)

RN 248937-34-0 CAPLUS

CN Gold, dichloro[1-[(2-pyrimidinyl-κN1)amino]-2-naphthalenyl-κC]-, (SP-4-3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:76937 CAPLUS

DOCUMENT NUMBER: 130:223399

TITLE: Cyclometallation of 2-(2-pyridyl)benzo[b]furan and 1-(2-pyridyl and 2-pyrimidyl)indole with palladium(II) and rhodium(III). Structures of unexpectedly formed nitro palladium(II) complexes

AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Nagoya, 464-8602, Japan

SOURCE: Polyhedron (1998), Volume Date 1999, 18(3-4), 533-543

CODEN: PLYHDE; ISSN: 0277-5387

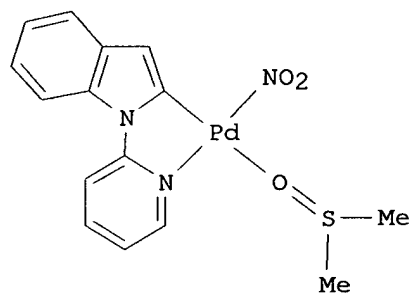
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

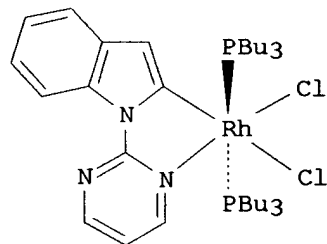
LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:223399

GI



I



II

AB Reactions of 2-(2-pyridyl)benzo[b]furan (Hpbfb), 1-(2-pyridyl)indole (Hpyi) and 1-(2-pyrimidyl)indole (Hpimi) with palladium(II) acetate in refluxing acetonitrile resulted in the formation of unexpected nitro complexes, $[\text{Pd}(\text{NO}_2)\text{L}(\text{CH}_3\text{CN})]$ ($\text{L} = \text{pbfb}$, pyi and pimi). The presence of NO_2 in the square planar DMSO (DMSO) derivs., $[\text{Pd}(\text{NO}_2)\text{L}(\text{DMSO})]$ ($\text{L} = \text{pbfb}$ and pyi I) were confirmed by X-ray anal. Palladation occurred at the C-3 of pbfb and at the C-2 of pyi and pimi and a five member palladacycle was formed. The NO_2 was coordinated trans to the pyridine-N atom and the DMSO trans to the C atom through the O atom. Cyclorhodation of Hpbfb, Hpyi and Hpimi with

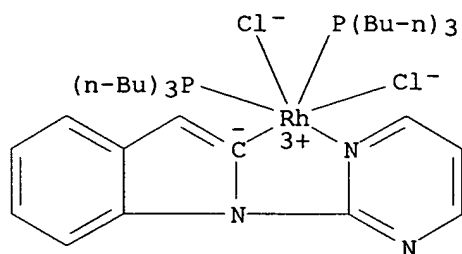
trichlorobis(tri-n-butylphosphine)rhodium(III) similarly occurred in refluxing toluene to afford octahedral complexes, $[\text{RhCl}_2\text{L}(\text{PBu}_3)_2]$, ($\text{PBu}_3 =$ tri-n-butylphosphine). The octahedral structure of $[\text{RhCl}_2(\text{pmi})(\text{PBu}_3)_2]$ II was also determined by X-ray anal. The two PBu_3 ligands were coordinated trans to each other and the strong trans influence of the $\sigma\text{-C}$ donor atom stretched one Rh-Cl bond trans to it.

IT **221043-97-6P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 221043-97-6 CAPLUS

CN Rhodium, dichloro[1-(2-pyrimidinyl- κN1)-1H-indol-2-yl- κC]bis(tributylphosphine)-, (OC-6-43)- (9CI) (CA INDEX NAME)

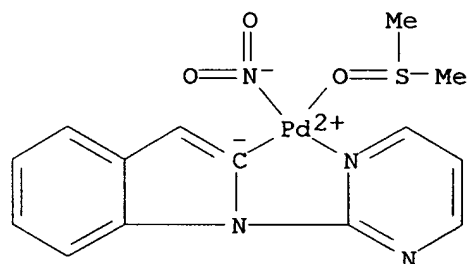


IT **221044-00-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 221044-00-4 CAPLUS

CN Palladium, (nitrito- κN)[1-(2-pyrimidinyl- κN1)-1H-indol-2-yl- κC] [(sulfinyl- κO)bis[methane]]-, (SP-4-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L4~~ ANSWER 6 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:316605 CAPLUS

DOCUMENT NUMBER: 129:35688

TITLE: Synthesis and characterization of Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Cr(III), Fe(III), Ru(III) and Rh(III) complexes with 1,1'-(2,6-pyrimidinediyl)bis(benzothiazole-2-thione)

AUTHOR(S): Khan, Tabrez A.; Shahjahan; Zaidi, S. A. A.

CORPORATE SOURCE: Dep. Chemistry, Jamia Millia Islamia, New Delhi, 110 025, India

SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (1998), 37A(2), 161-164
CODEN: ICACEC; ISSN: 0376-4710

PUBLISHER: National Institute of Science Communication, CSIR

DOCUMENT TYPE: Journal

LANGUAGE: English

AB M(PBT)2Cl₂ and M'(PBT)2Cl₆ (PBT = 1,1'-(2,6-pyrimidinediyl)bis(benzothiazole-2-thione); M = Mn, Co, Ni, Cu, Zn and M' = Cr, Fe, Ru, Rh) were synthesized and characterized by elemental anal., magnetic susceptibility, IR, ¹H NMR and electronic spectral studies. The ligand coordinates through pyrimidine N and thiocarbonyl S atoms of the mercaptobenzothiazolyl group. M(PBT)2Cl₂ complexes appear to be octahedral whereas M'(PBT)2Cl₆ complexes probably have a Cl-bridged dimeric octahedral structure.

IT 208044-98-8P 208044-99-9P 208045-00-5P

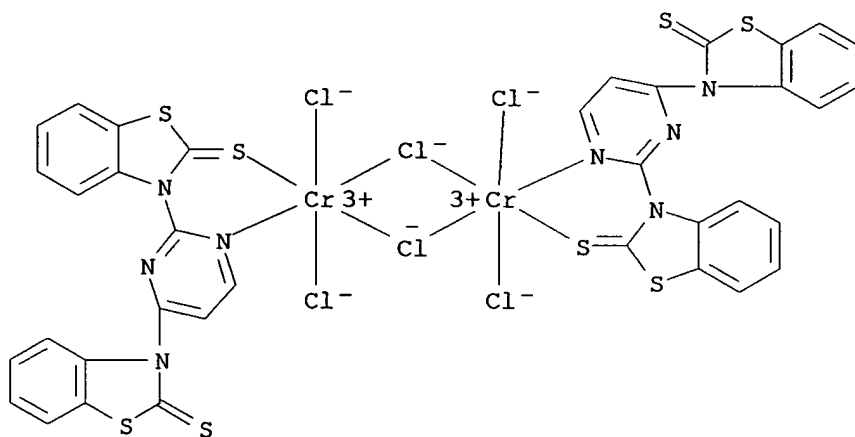
208045-01-6P 208045-02-7P 208045-03-8P

208045-04-9P 208045-05-0P 208045-06-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

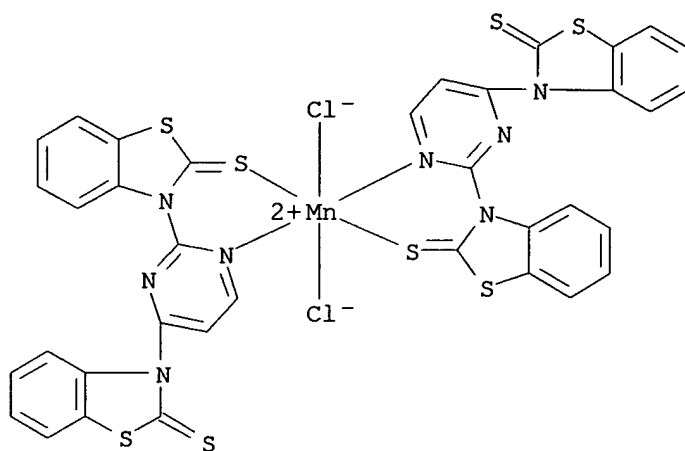
RN 208044-98-8 CAPLUS

CN Chromium, di-μ-chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



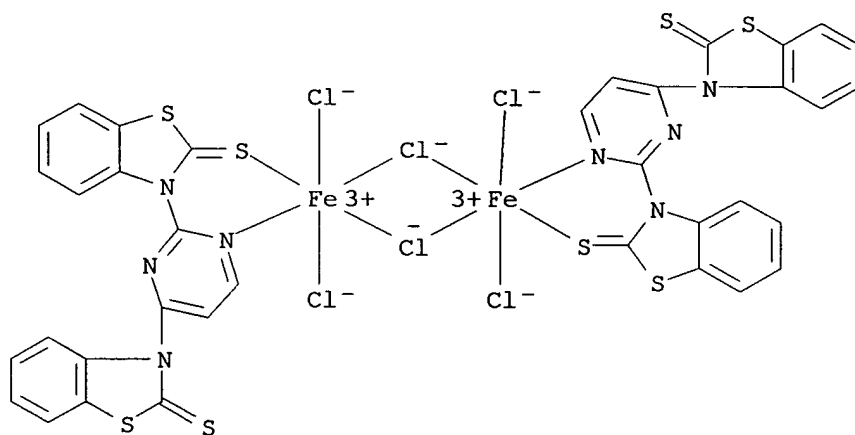
RN 208044-99-9 CAPLUS

CN Manganese, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



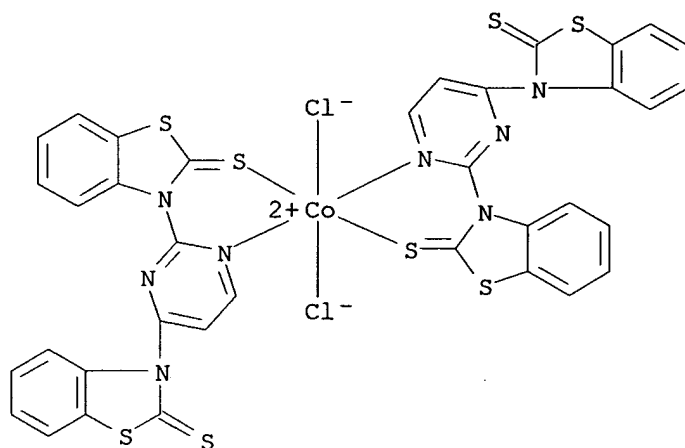
RN 208045-00-5 CAPLUS

CN Iron, di- μ -chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl- κ N1]-2(3H)-benzothiazolethione- κ S2]di- (9CI) (CA INDEX NAME)



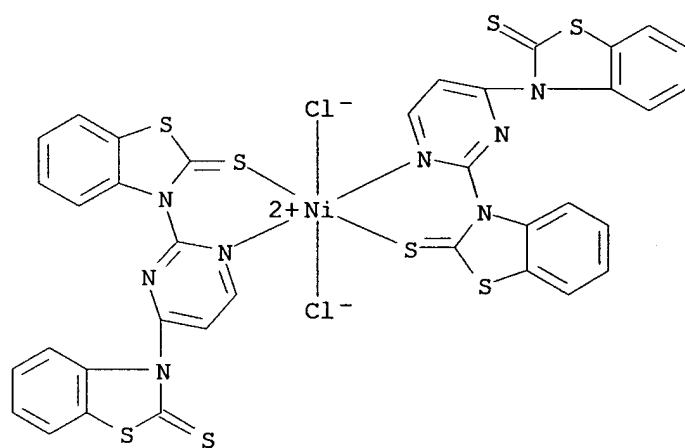
RN 208045-01-6 CAPLUS

CN Cobalt, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl- κ N1]-2(3H)-benzothiazolethione- κ S2]di- (9CI) (CA INDEX NAME)



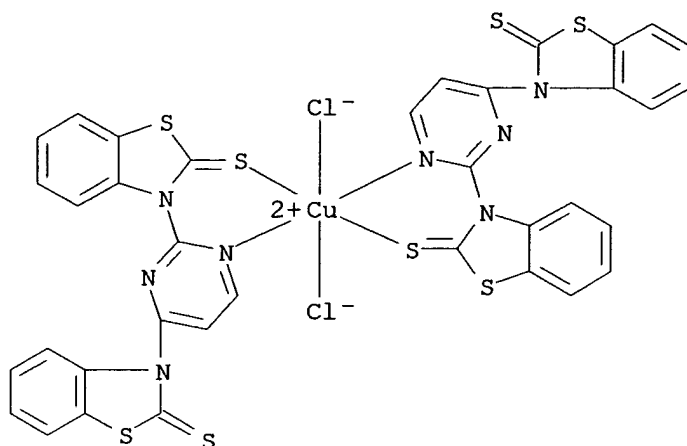
RN 208045-02-7 CAPLUS

CN Nickel, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



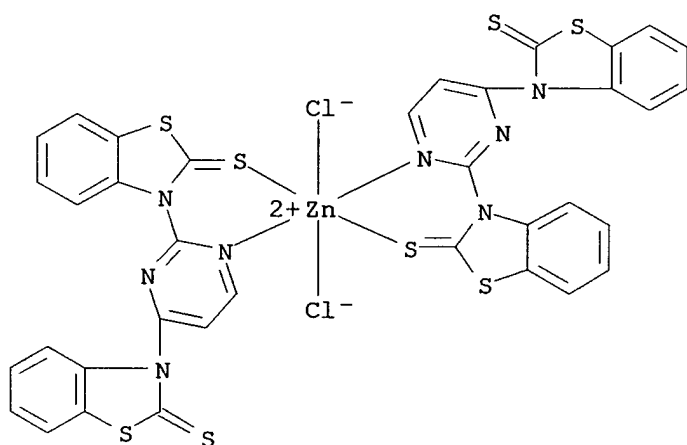
RN 208045-03-8 CAPLUS

CN Copper, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



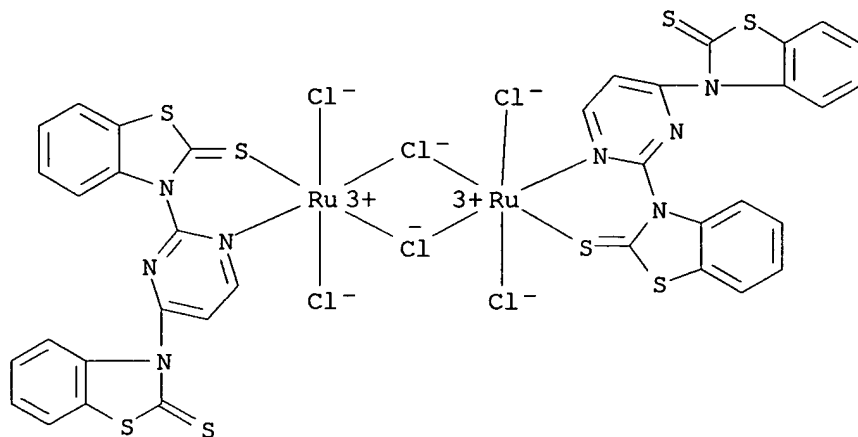
RN 208045-04-9 CAPLUS

CN Zinc, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl- κ N1]-2(3H)-benzothiazolethione- κ S2]di- (9CI) (CA INDEX NAME)



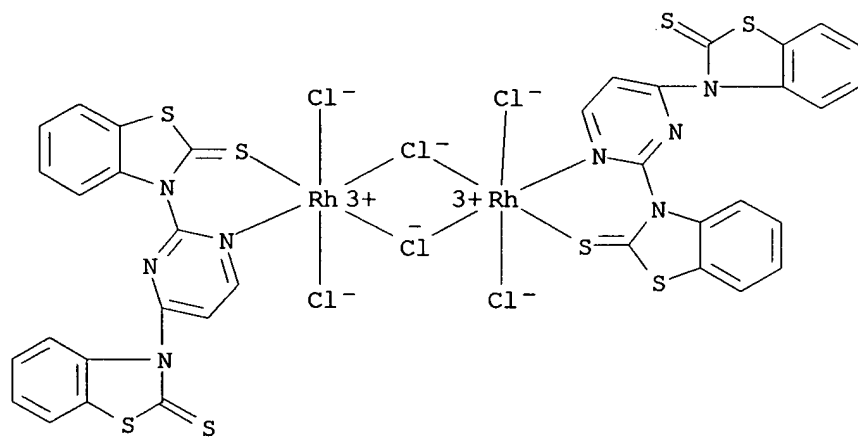
RN 208045-05-0 CAPLUS

CN Ruthenium, di- μ -chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl- κ N1]-2(3H)-benzothiazolethione- κ S2]di- (9CI) (CA INDEX NAME)



RN 208045-06-1 CAPLUS

CN Rhodium, di- μ -chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl- κ N1]-2(3H)-benzothiazolethione- κ S2]di- (9CI)
(CA INDEX NAME)



REFERENCE COUNT:

14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/644,076

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:707745 CAPLUS

DOCUMENT NUMBER: 128:3751

TITLE: Direct cycloauration of 2-anilinopyridine (Hanp) with tetrachloroaurate(III) and the X-ray crystal structure of [AuCl₂(anp)]

AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko; Nonoyama, Kiyoko
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Chikusa, 464-01, Japan

SOURCE: Polyhedron (1997), 16(23), 4039-4044
CODEN: PLYHDE; ISSN: 0277-5387

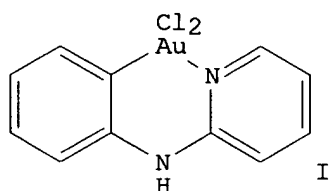
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:3751

GI



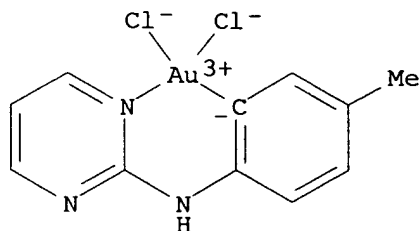
AB 2-Anilinopyridine (Hanp) reacted with Na tetrachloroaurate(III) in refluxing H₂O directly to give cyclometalated [AuCl₂(anp)] I, which was characterized spectroscopically and its structure determined by x-ray anal. The metalation reaction involved direct activation of an ortho C-H bond of the Ph moiety and the deprotonated anionic ligand, anp, coordinated to Au through the pyridine-N and Ph ortho-C atoms forming a six-membered chelate ring. Similarly cycloaurated complexes, [AuBr₂(anp)] and [AuCl₂(C-N)] (CN = tlp, map, and tpm), were also prepared and characterized [Htlp = 2-(p-toluidino)pyridine, Hmap = 2-(N-methylanilino)pyridine, and Htpm = 2-(p-toluidino)pyrimidine].

IT 198711-23-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(direct cycloauration of anilinopyridine and related compds. with tetrachloroaurate)

RN 198711-23-8 CAPLUS

CN Gold, dichloro[5-methyl-2-[(2-pyrimidinyl-κN1)amino]phenyl-κC]-, (SP-4-3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~14~~ ANSWER 8 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:419210 CAPLUS

DOCUMENT NUMBER: 119:19210

TITLE: Coordination properties of new indazole derivatives

AUTHOR(S): Zaidi, Saiyid Aftab Ahmad; Shahjahan; Siddiqui, Khwaja Salahuddin

CORPORATE SOURCE: Dep. Chem., Aligarh Muslim Univ., Aligarh, 202 002, India

SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands) (1993), 18(1), 51-4

CODEN: TMCHDN; ISSN: 0340-4285

DOCUMENT TYPE: Journal

LANGUAGE: English

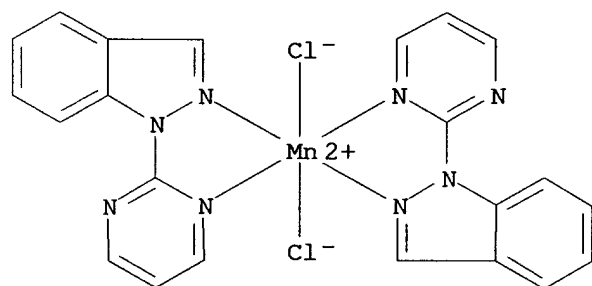
AB The bidentate N donor ligands (L) 2-(1-indazolyl)pyridine and 2-(1-indazolyl)pyrimidine were synthesized. ML_2Cl_2 (M = Mn, Co, Ni, Cu, Zn) were prepared and characterized by elemental anal., IR, UV spectra, and magnetic susceptibilities. The complexes are nonelectrolytes and have magnetic moments consistent with an octahedral environment.

IT **148099-98-3P 148099-99-4P 148100-20-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR and UV spectra and crystal field parameters and reaction of, with pyridine)

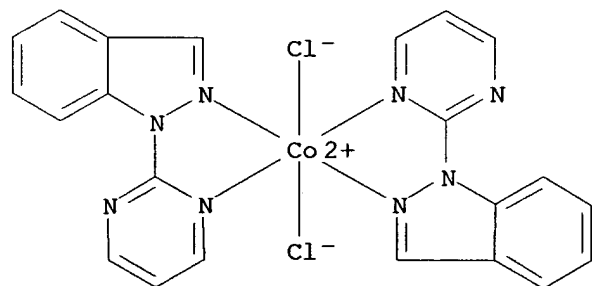
RN 148099-98-3 CAPLUS

CN Manganese, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)



RN 148099-99-4 CAPLUS

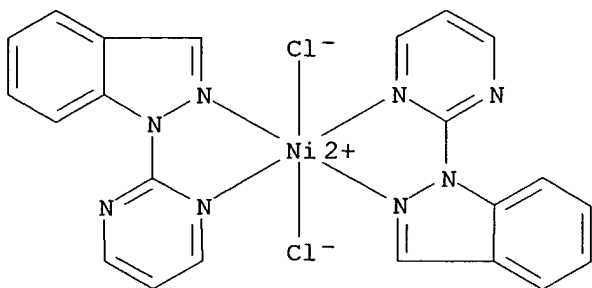
CN Cobalt, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)



RN 148100-20-3 CAPLUS

CN Nickel, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA

INDEX NAME)

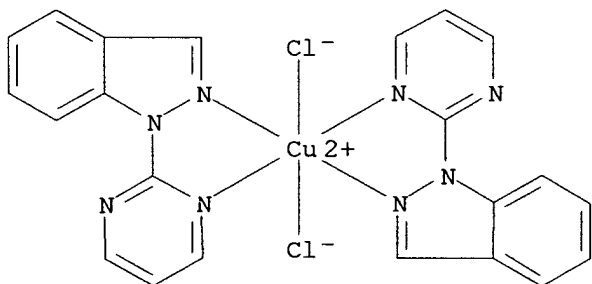
IT **148100-21-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and IR and UV spectra and reaction of, with pyridine)

RN 148100-21-4 CAPLUS

CN Copper, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)

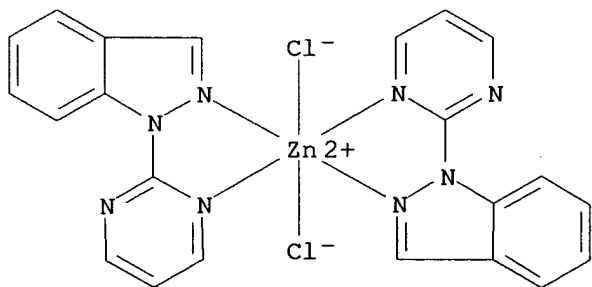
IT **148100-22-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)

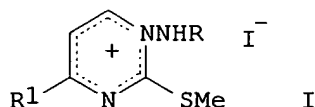
(preparation and IR spectrum and reaction of, with pyridine)

RN 148100-22-5 CAPLUS

CN Zinc, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)

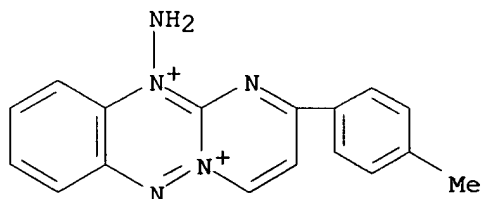


ANSWER 9 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1990:235255 CAPLUS
 DOCUMENT NUMBER: 112:235255
 TITLE: 1-Amino-2-hydrazinopyrimidine N-ylides. Unusual
 tautomers of 1-aminopyrimidine 2-hydrazones
 AUTHOR(S): Liebscher, Juergen; Hassoun, Ahmed; Fabian, Juergen
 CORPORATE SOURCE: Sek. Chem., Humboldt-Univ. Berlin, Berlin, DDR-1040,
 Ger. Dem. Rep.
 SOURCE: Monatshefte fuer Chemie (1989), 120(8-9), 749-58
 CODEN: MOCMB7; ISSN: 0026-9247
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 112:235255
 GI



AB 1-Amino-2-methylthiopyrimidin-5-ium iodides I [R = Ph, C₆H₅, 4-O₂NC₆H₄,
 2,4-(O₂N)₂C₆H₃, Ac; R₁ = Ph, 4-MeC₆H₄, 4-ClC₆H₄, 4-MeOC₆H₄] were prepared by
 reaction of 3-isothiocyanato-2-propeniminium perchlorates with hydrazines
 and subsequent methylation of the resulting 1-amino-2(1H)-
 pyrimidinethiones. Reaction of I with hydrazine causes substitution of
 the methylthio group and results in the formation of deeply colored
 1-amino-2-hydrazinopyrimidine N-ylides as unusual tautomers of the
 commonly expected 1-amino-2(1H)-pyrimidine hydrazones. The structure of
 these N-ylides was proved by spectroscopic methods as well as by
 subsequent transformation to 3-amino-1,2,4-triazole[2,3-a]pyrimidin-5-ium
 salts by dehydration or to pyrimidotriazin-5-ium salt by oxidation. Reaction of
 N,N-disubstituted 1-amino-2-methylthiopyrimidin-5-ium salt with hydrazine
 also causes substitution of methylthiol; the resulting orange
 N,N-disubstituted 1-amino-2(1H)-pyrimidine hydrazone, however, cannot
 tautomerize to N-ylides.

IT **127252-20-4P 127252-22-6P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 127252-20-4 CAPLUS
 CN Pyrimido[1,2-b][1,2,4]benzotriazin-5-ium, 11-amino-2-(4-methylphenyl)-,
 dibromide (9CI) (CA INDEX NAME)



● 2 Br⁻

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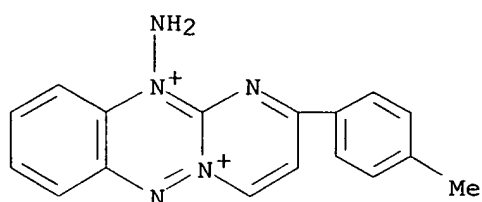
RN 127252-22-6 CAPLUS

CN Pyrimido[1,2-b][1,2,4]benzotriazin-5-ium, 11-amino-2-(4-methylphenyl)-,
diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 127252-21-5

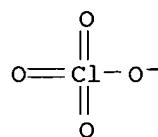
CMF C17 H15 N5



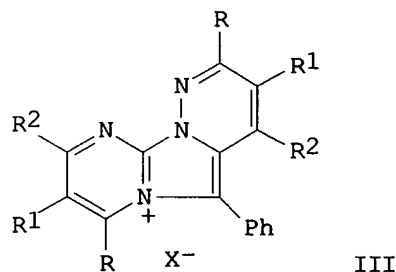
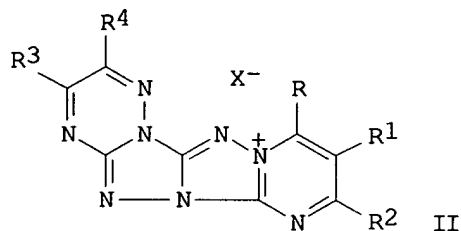
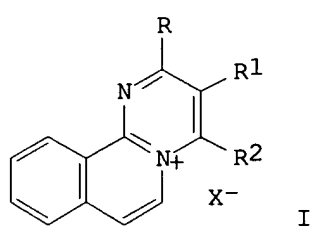
CM 2

CRN 14797-73-0

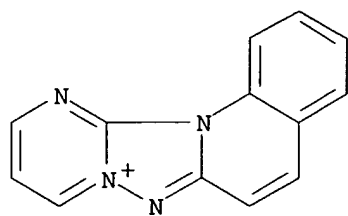
CMF Cl O4



14 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1976:544683 CAPLUS
 DOCUMENT NUMBER: 85:144683
 TITLE: Condensed pyrimidinium salts derived from
 isoquinoline, condensed s-triazoles, and imidazole
 AUTHOR(S): Nuiguk, V. A.; Golubushina, G. M.; Bachkovskii, I. P.;
 Fedotov, K. V.
 CORPORATE SOURCE: Kiev. Univ. im. Shevchenko, Kiev, USSR
 SOURCE: Tezisy Dokl. - Simp. Khim. Tekhnol. Geterotsikl.
 Soedin. Goryuch. Iskop., 2nd (1973), 17-18. Donetsk.
 Gos. Univ.: Donetsk, USSR.
 CODEN: 33XLA8
 DOCUMENT TYPE: Conference
 LANGUAGE: Russian
 GI



AB Condensation of 1-aminoisoquinoline-HClO₄ [53686-45-6] with RCOCHR₁COR₂ or the related β -chlorovinyl ketones gave I. Analogous reactions with 1-amino-s-triazolo[4,3-a]quinoline [41569-09-9], 3-amino-s-triazolo[4,3-b]pyridazine [53854-45-8], or 3-amino-s-triazolo[3,4-a]phthalazine [21517-08-8] gave the resp. condensed pyrimidinium salts. Condensation of 3,6,7-triamino-7H-s-triazolo[4,3-b]-s-triazole [13728-15-9] with RCOCHR₁COR₂ and R₃COCOR₄ gave II via the intermediates with only 1 ring added. Condensation of 1,2-diamino-4-phenylimidazole [15970-40-8] with 2 moles RCOCHR₁COR₂ gave III. Any of these condensed pyrimidinium salts with R, R₁, or R₂ = Me could be converted to cyanines.
 IT **54063-69-3DP**, Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, derivs.
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 54063-69-3 CAPLUS
 CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium (9CI) (CA INDEX NAME)



10/644,076

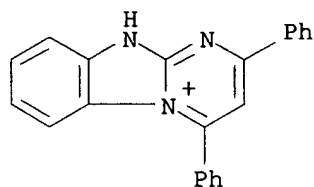
14 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:74304 CAPLUS
DOCUMENT NUMBER: 84:74304
TITLE: 1,3-Diphenylpyrimido[1,2-a]benzimidazolium
perchlorates
INVENTOR(S): Zvezdina, E. A.; Dorofeenko, G. N.; Zhdanova, M. P.;
Simonov, A. M.
PATENT ASSIGNEE(S): Rostov State University, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,
Tovarnye Znaki 1975, 52(41), 97.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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SU 490801	T	19751105	SU 1974-1993642	19740129

PRIORITY APPLN. INFO.: SU 1974-1993642 A 19740129
GI For diagram(s), see printed CA Issue.
AB The title compds. I (R = lower alkyl or aralkyl; R1 = H, Me) were prepared
by treatment of 2-aminobenzimidazoles with 2,4,6-triphenylpyrylium
perchlorate in absolute DMF at reflux.
IT **58537-58-9DP**, 10H-Pyrimido[1,2-a]benzimidazol-5-ium,
2,4-diphenyl-, perchlorate, derivs. **58537-60-3DP**,
10H-Pyrimido[1,2-a]benzimidazol-5-ium, 7,8-dimethyl-2,4-diphenyl-,
perchlorate, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58537-58-9 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-diphenyl-, perchlorate (9CI)
(CA INDEX NAME)

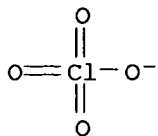
CM 1

CRN 58537-57-8
CMF C22 H16 N3



CM 2

CRN 14797-73-0
CMF C1 O4



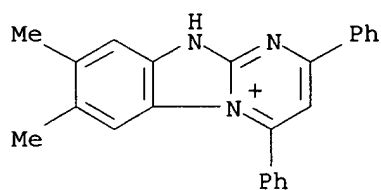
RN 58537-60-3 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 7,8-dimethyl-2,4-diphenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 58537-59-0

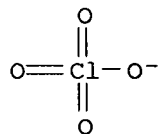
CMF C24 H20 N3



CM 2

CRN 14797-73-0

CMF Cl O4



ACCESSION NUMBER: 1974:552154 CAPLUS

DOCUMENT NUMBER: 81:152154

TITLE: New heterocyclic systems of S-triazolopyrimidinium derivatives of quinoline, pyridazine, and phthalazine

AUTHOR(S): Golubushina, G. M.; Ponomarenko, O. G.; Poshtaruk, G. N.; Chuiguk, V. A.

CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR

CODEN: KGSSAQ; ISSN: 0132-6244

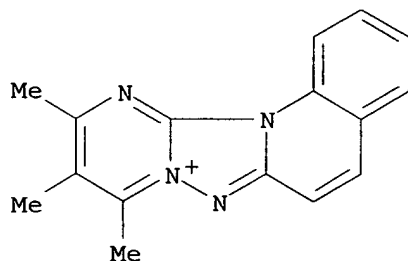
LANGUAGE: Russian

AB Pyrimido-triazolopyridazinium perchlorates (I; R1 = H, Cl, R2 = H, Me; R3 = Me, H; R4 = Me, Ph, H) were obtained in 39-100% yields by condensation of a β -diketone with an aminotriazolopyridazine in F3CCO2H.

IT 53854-43-6P 53854-44-7P 53890-38-3P

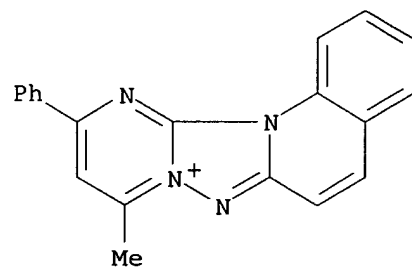
RN 53854-43-6 CAPLUS

CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium,
9,10,11-trimethyl-, iodide (9CI) (CA INDEX NAME)



● T-

CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium,
9-methyl-11-phenyl-, bromide (9CI) (CA INDEX NAME)



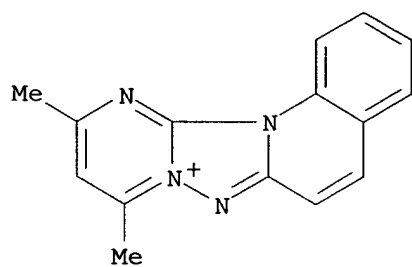
RN 53890-38-3 CAPLUS

CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, 9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 53890-37-2

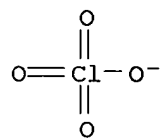
CMF C15 H13 N4



CM 2

CRN 14797-73-0

CMF C1 O4



10/644,076

~~L4~~ ANSWER 13 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:488425 CAPLUS

DOCUMENT NUMBER: 77:88425

TITLE: Condensation of 2-amino-3,4,5,6-tetrahydroimidazo
[4,5,1-ij]quinoline and 2-amino-2-pyrrole with
 β -diketones

AUTHOR(S): Golubushina, G. M.; Chuiguk, V. A.

CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (3),
419-21

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB 2-Amino-3,4,5,6-tetrahydroimidazo[4,5,1-ij]-quinoline perchlorate when
heated 2 hr at 180-90° with β -diketones gave five

1,2,3,12-tetrahydropyrimido[2, 1 :2,3]imidazo-[4,5,1-ij]quinolinium
perchlorates (I, R, R1, R2 = H, Me, Ph, Et) in yields of 18-58%.

4-Methyl-7,8-dihydro-6H-pyrrolo[1,2-a]pyrimidinium perchlorates (II, R =
Me, Ph) were similarly prepared in 20-27% yield.

IT **38340-23-7P 38340-24-8P 38340-70-4P**

38340-71-5P 38340-72-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

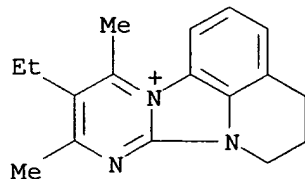
RN 38340-23-7 CAPLUS

CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium,
10-ethyl-5,6-dihydro-9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 47045-38-5

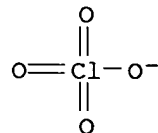
CMF C17 H20 N3



CM 2

CRN 14797-73-0

CMF C1 O4



RN 38340-24-8 CAPLUS

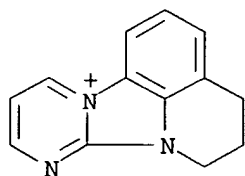
10/644,076

CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46487-03-0

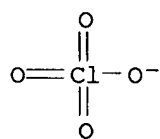
CMF C13 H12 N3



CM 2

CRN 14797-73-0

CMF C1 O4



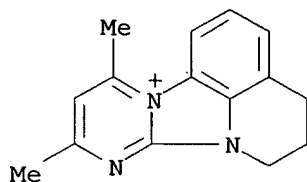
RN 38340-70-4 CAPLUS

CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46864-77-1

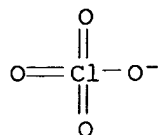
CMF C15 H16 N3



CM 2

CRN 14797-73-0

CMF C1 O4

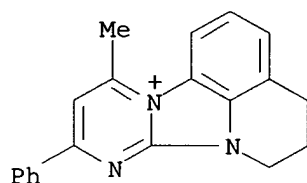


RN 38340-71-5 CAPLUS
 CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium,
 5,6-dihydro-11-methyl-9-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 47286-43-1

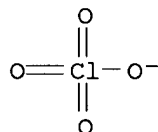
CMF C20 H18 N3



CM 2

CRN 14797-73-0

CMF Cl O4



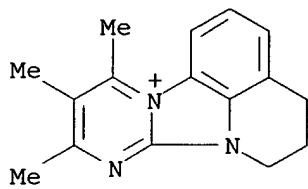
RN 38340-72-6 CAPLUS
 CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium,
 5,6-dihydro-9,10,11-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46960-85-4

CMF C16 H18 N3

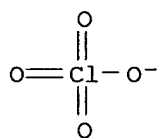
10/644,076



CM 2

CRN 14797-73-0

CMF Cl O4



~~DA~~ ANSWER 14 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:59508 CAPLUS

DOCUMENT NUMBER: 76:59508

TITLE: Synthesis and pharmacological properties of some new condensed derivatives of benzothiazoline thiazolo, and benzothiazolopyrimidine

AUTHOR(S): Lisunkin, Yu. I.; Chuiguk, V. A.

CORPORATE SOURCE: Kiev Res. Inst. Pharmacol. Toxicol., Kiev, USSR

SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1971), 26(5), 20-5
CODEN: FRZKAP; ISSN: 0367-3057

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

AB 2-Amino- and 1-methyl-2-amino-2-imidazoline-HBr and -thiazole-HBr, 2-amino-4-phenylthiazole-HBr, 2-aminobenzothiazole-HBr, and 1-methyl-2-aminobenzimidazole-HBr condensed with Ac₂CH₂ to give the corresponding condensed-ring heterocyclic pyrimidinium salts in 39-95% yield. 3a,9-Dimethyl- and 3a-methyl-1,2,3,3a-tetrahydropyrrolo[2,1-b]benzothiazolium chloride and 4a-methyl-1,2,3,4,4a,10-hexahydro[2,1-b]benzothiazolium and -benzoxazolium bromide were prepared analogously using O-H₂NC₆H₆OH and O-H₂NC₆H₄SH derivs. These compds. exerted a hypotensive effect when administered i.v. to mice, but did not affect pain sensitivity or the duration of barbiturate or chloral hydrate narcosis; LD₅₀ values were 38-385 mg/kg body weight Arecoline and nicotine hyperkinesis in mice were ptentiated; the sensitivity of frog transverse abdominal muscle to acetylcholine was reduced.

IT 35220-93-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

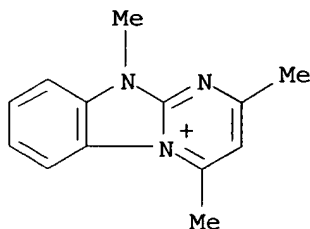
RN 35220-93-0 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4,10-trimethyl-, perchlorate
(9CI) (CA INDEX NAME)

CM 1

CRN 46496-90-6

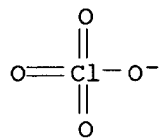
CMF C13 H14 N3



CM 2

CRN 14797-73-0

CMF C1 O4



ANSWER 15 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:46158 CAPLUS

DOCUMENT NUMBER: 76:46158

TITLE: Condensation of salts of 2-aminobenzimidazoles with β -diketones and β -chlorovinyl ketones

AUTHOR(S): Golubushina, G. M.; Chuiguk, V. A.

CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR

SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1971), 37(11), 1132-4

CODEN: UKZHAU; ISSN: 0041-6045

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB Salts of 2-amino-1-methyl- and 2-amino-1-phenylbenzimidazole were condensed with β -diketones and β -chlorovinyl ketones to form 8 quaternary salts of structure I (R=Me or Ph, R1 and R3=H or Me, and R2=Me, Et, or Ph). Some of these compds. were identical with the quaternary salts obtained from pyrimido[1,2-a]benzimidazoles (CA 59: 15411c) which indicates that the latter do not have structure II.

IT 35220-93-0P 35220-95-2P 35220-96-3P

35220-97-4P 35220-98-5P 35220-99-6P

35221-00-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

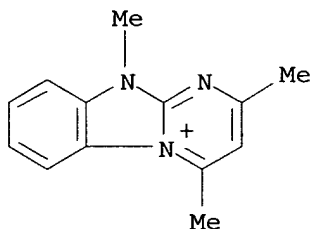
RN 35220-93-0 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4,10-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46496-90-6

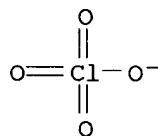
CMF C13 H14 N3



CM 2

CRN 14797-73-0

CMF Cl O4



10/644,076

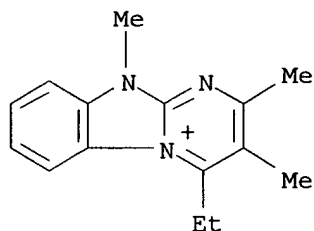
RN 35220-95-2 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-ethyl-2,3,10-trimethyl-,
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46864-34-0

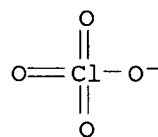
CMF C15 H18 N3



CM 2

CRN 14797-73-0

CMF Cl O4



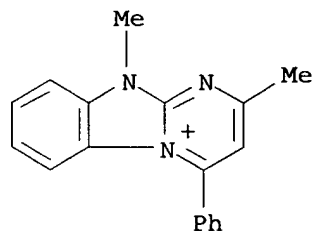
RN 35220-96-3 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,10-dimethyl-4-phenyl-,
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 47127-07-1

CMF C18 H16 N3

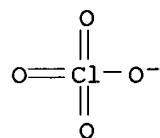


CM 2

CRN 14797-73-0

10/644,076

CMF Cl O4



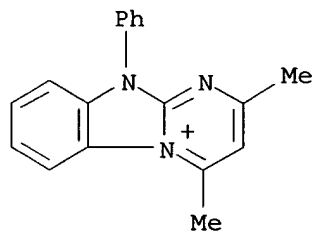
RN 35220-97-4 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-dimethyl-10-phenyl-, salt with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 47127-37-7

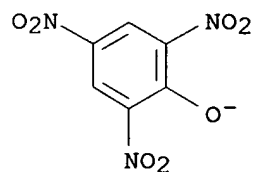
CMF C18 H16 N3



CM 2

CRN 14798-26-6

CMF C6 H2 N3 O7



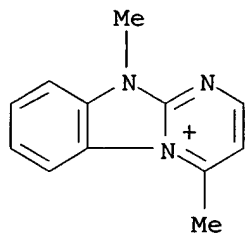
RN 35220-98-5 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4,10-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46388-80-1

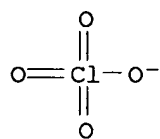
CMF C12 H12 N3



CM 2

CRN 14797-73-0

CMF Cl O4



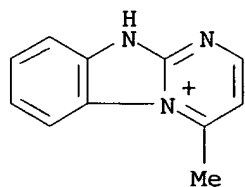
RN 35220-99-6 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-methyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46266-98-2

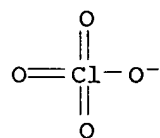
CMF C11 H10 N3



CM 2

CRN 14797-73-0

CMF Cl O4



10/644,076

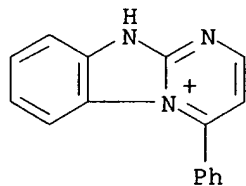
RN 35221-00-2 CAPLUS

CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46955-67-3

CMF C16 H12 N3



CM 2

CRN 14797-73-0

CMF C1 O4

